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14. ABSTRACT

The present program is concerned with the dynamics of droplet collision and flame-flow interaction that are of relevance to liquid-fueled turbulent combustion in high-pressure propulsive devices. The investigation during the reporting period involved six projects, namely: (1) Formulation of a comprehensive theory of the dynamics of binary droplet collision, especially in predicting the experimentally observed bouncing and coalescence phenomena; (2) Computational investigation of the gasification mechanism of multicomponent droplets, demonstrating that at elevated pressures the influence of liquid-phase mass diffusion is weakened; (3) A comprehensive study on the influence of elevated pressure on chemical kinetics; (4) Formulation of a theory of acoustic-flame resonance; (5) transition to detonation of an accelerating expanding flame; (6) computational simulation of the flame stabilization in a nozzle-generated flow.

15. SUBJECT TERMS
Droplet collision; van der Waals force; multicomponent droplets; fuel distillation; fuel oxidation mechanisms; high-pressure kinetics; flamefront hydrodynamic and body-force instabilities; flame acceleration; deflagration-to-detonation transition; flame stabilization.

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Final Technical Report

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DROPLET AND SUPERCRITICAL FLAME DYNAMICS IN PROPULSION

(AFOSR FA9550-06-1-0094)

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BACKGROUND

This research program aimed to investigate several major thrusts concerning droplet and supercritical flame processes in high-pressure environments, with particular interest on understanding and quantifying the cause and control of combustion instability in rocket engines. During the reporting period, we have studied droplet-droplet and droplet-film collision, gasification characteristics of multicomponent droplets in sub- and supercritical environments, and the effect of elevated pressure on chemical kinetics. In addition, we have investigated the dynamics and stability of flames, namely, the combustion instability induced by flame-acoustic interactions, the transition to detonation of an accelerating expanding flame, and the stabilization of a turbulent flame downstream of an injection nozzle. High-lights of the research accomplishments are presented in the following.

RESEARCH ACCOMLISHMENTS

1. Droplet-Droplet Collision

We have formulated a comprehensive theory on the head-on collision of two identical droplets, with the attendant bouncing and coalescence outcomes, for situations when the extent of droplet deformation upon collision is comparable to the original droplet radius. The theory embodies the essential physics that describes the substantial amount of droplet deformation for even moderately large collision Weber numbers, *We*, the viscous loss through droplet internal motion, the dynamics and rarefied nature of the gas film between the interfaces of the colliding droplets, and the potential destruction and thereby merging of these interfaces due to the van der Waals attraction force. Figure 1 shows a schematic of the components of the theory. The theoretical results agree well with previous experimental observations in that as the impact inertia increases, droplet collision results in the nonmonotonic outcomes of coalescence, bouncing, and coalescence again, that bouncing is promoted with increasing ambient pressure, and that alkane droplets are more susceptible to bouncing than water droplets.

This work has been submitted for publication considerations under the title: “Theory of bouncing and coalescence in head-on droplet collision with large deformation”, see Publication #1.

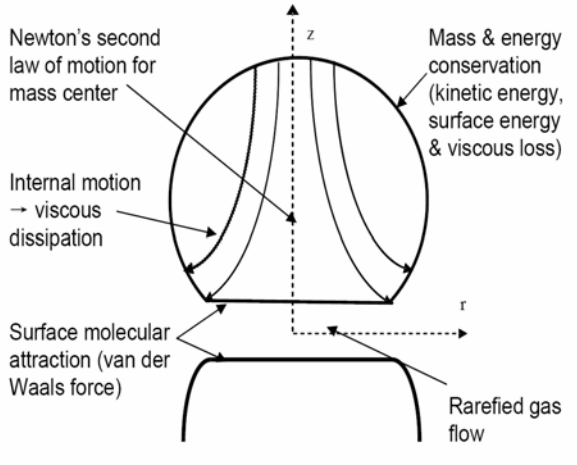


Figure 1.

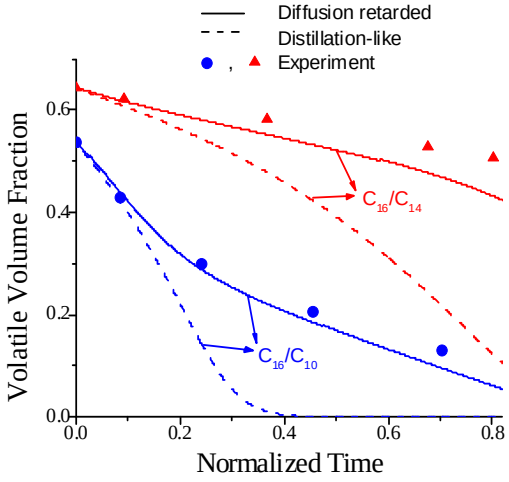


Figure 2.

2. Theory of Multicomponent Droplet Gasification

In this study we have considered the relative roles of liquid-phase diffusional resistance and volatility differential in multicomponent droplet gasification, recognizing that liquid-phase mass diffusivities can be substantially increased as the droplet is progressively heated upon initiation of gasification, leading to a corresponding substantial weakening of the diffusional resistance. Calculations performed by using realistic and temperature-dependent thermal and mass diffusivities indeed substantiate this influence. In particular, the calculated results agree with the literature experimental data, indicating that the gasification mechanism of multicomponent fuels is intermediate of diffusion and distillation limits as demonstrated in Fig. 2. We have also investigated gasification at elevated pressures, recognizing that the liquid boiling point and hence the attainable droplet temperature would increase with increasing pressure, causing further weakening of the liquid-phase diffusional resistance. This possibility was again verified through computational results, suggesting further departure from the diffusion limit toward the distillation limit behavior for gasification at high pressures. It is also found that diffusional resistance is stronger for the lighter, gasoline-like fuels as compared to the heavier, diesel-like fuels because the former have overall lower boiling points, lower attainable droplet temperatures, and hence lower mass diffusivities in spite of their smaller molecular weights.

This work has been published in *Combustion and Flame* **153**, 593-602 (2008); see Publication #2.

3. High-Pressure Chemical Kinetics

While there are situations for which chemistry may not be important in combustion phenomena, such as the diffusion-controlled steady burning, accounting for chemical kinetics is inherently important for such critical events as ignition and extinction. Furthermore, it is now well established that the chemistry governing fuels oxidation is usually very complex, with mechanisms involving tens to hundreds and thousands of species and hundreds to ten thousands of reactions. In addition, the rates of these reactions are highly sensitive functions of temperature and pressure, which can also span over many orders of magnitude. Consequently it is basically impossible to include detailed chemistry in the simulation of combustion phenomena, except for such small fuel molecules as hydrogen and methane, and for such simple phenomena as the one-dimensional flame.

In order to accommodate some measure of the influence of chemistry, one-step overall reaction with constant kinetic parameters is frequently used in either computational simulation or theoretical analysis. Such an approximation, however, is highly unsatisfactory, as demonstrated in Figs. 3 and 4, which show the variations of the overall reaction order and activation energy governing the propagation of the planar laminar flame propagation with increasing pressure, for H_2-O_2 and CH_4-O_2 mixtures respectively. It is clearly seen that these two parameters vary substantially with pressure, and as such would induce serious quantitative error if assumed to be constants.

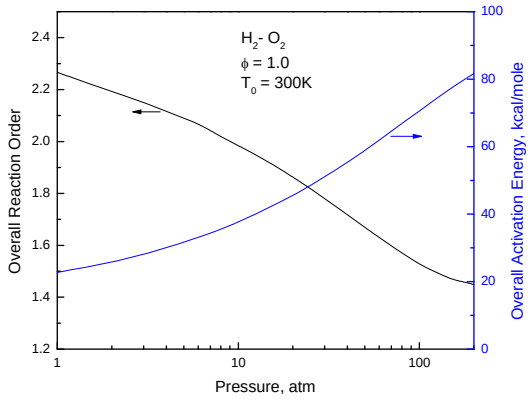


Figure 3.

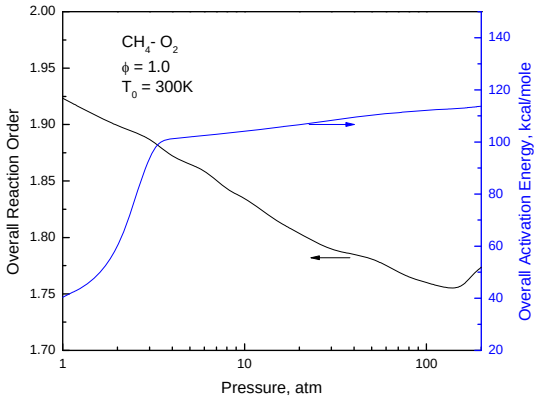


Figure 4.

It is also tempting to explore if some simplification can be made by restricting the thermodynamic states of the mixture, for example by specializing to high pressure situations. Figure 5 shows the error induced by neglecting one of the reactants in the mechanism for the ignition of an H_2-O_2 mixture; generally an error greater than 0.1 is considered unacceptable. The results therefore show conclusively that the 8-species mechanism used is already the absolutely minimum that cannot be further reduced.

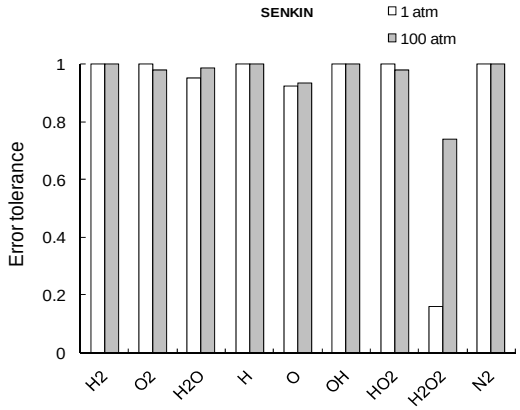


Figure 5.

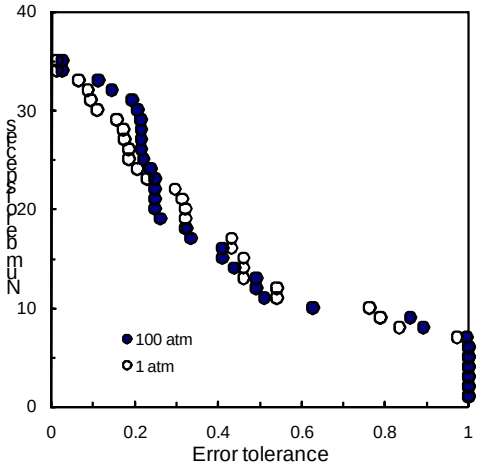


Figure 6

Figure 6 shows the error incurred with progressive reduction of the size of a CH_4-air mechanism. It is seen that the reduction curve for 1 and 100 atmosphere pressures track each other quite closely, with the reduction at 100 atmospheres being more difficult.

We have therefore demonstrated that the reaction mechanisms at high pressures are not simpler than those at the lower pressures, and as such should be kept if chemical fidelity is needed. This work is under preparation for publication considerations.

4. Theory of Combustion Instability through Flame-Acoustic Resonance

A systematic analysis was carried out for the interaction of a stable premixed flame in a duct with vortical perturbations superimposed on the oncoming mixture. Figure 7 shows a schematic of the problem analyzed. In the analysis a small-amplitude vortical perturbation with a frequency ω induces a hydrodynamic field in the vicinity of the flame and causes the initially flat flame to wrinkle. The unsteady heat release resulting from the increased surface area of the wrinkling flame then generates a sound wave with frequency of 2ω. When 2ω coincides with the natural frequency of an acoustic mode of the duct, a flame-

acoustic resonance takes place, through which the flame-induced sound may attain an amplitude that is sufficiently large to modulate the flame through the unsteady Rayleigh-Taylor effect. An evolution system is derived for the two-way coupling for a stationary flame with a fixed mean position, as well as for a moving flame. Numerical solution for the former situation shows that the mutual flame-acoustic interaction initiates a violent instability, and the flame-acoustic system quickly evolves into a fully nonlinear regime, which corresponds to a state of self-sustained oscillation. Thus a small-amplitude vortical perturbation may completely destabilize an otherwise stable flat flame. For the latter situation, the flame-acoustic resonance is of transient nature. The acoustic pressure gains substantially, but the flame instability is induced only when the vortical disturbance exceeds a finite threshold.

This work has been published in *Journal of Fluid Mechanics* **634**, 321–357 (2009); see Publication #3.

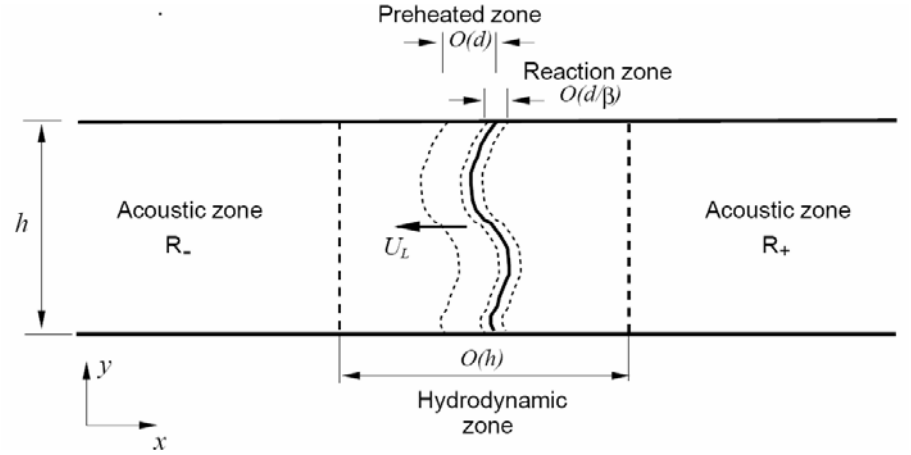


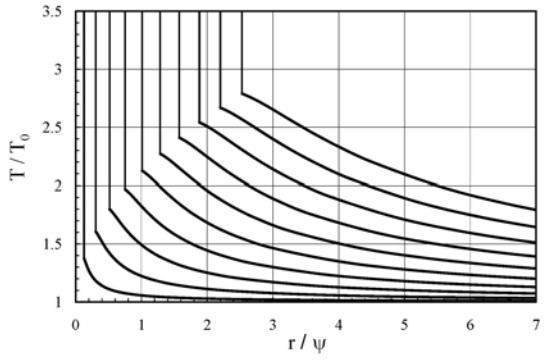
Figure 7.

5. Transition to Detonation of a Self-Accelerating Flame

While all flames are subjected to the hydrodynamic, Darrieus-Landau instability, the tendency is particularly strong at high pressures because of the reduced flame thickness. For an outwardly-expanding flame, the instability wrinkles the flame surface, causing an increase in its area and consequently the corresponding propagation rate. This could eventually lead to the transition to detonation. In this work we have developed a theory of explosion triggering by a centrally-ignited outwardly-propagating flame accelerating with $R_F = At^a$. The theory describes radial compression waves pushed by the flame, the

trajectories of gas particles, and the condition of explosion in the gas upstream of the flamefront. The instant and locus of explosion are determined for a given reaction mechanism. For induction time in the form of a Heaviside-like function, analytic expressions for the explosion time and position are derived, showing their dependence on the flame and flow parameters including thermal expansion, adiabatic exponent, and the acceleration rate of the flamefront. Figure 8 shows evolution of the temperature profile ahead of the flame. The instant and position of explosion versus the ignition temperature are presented in Fig. 9. Here φ and ψ are the characteristic time and length scales of the problem.

This work has been submitted for publication considerations under the title: “Self-similar accelerative propagation of expanding wrinkled flames and explosion triggering”; see Publication #4.



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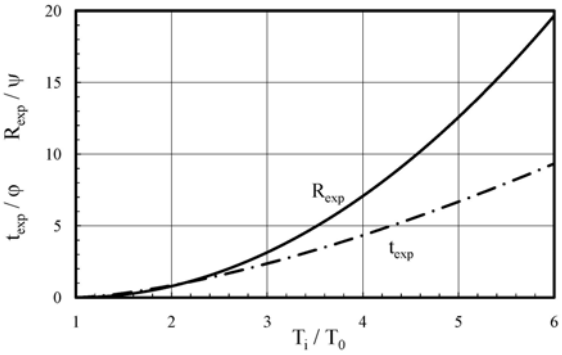

Figure 9.

6. Stabilization of Turbulent Lifted Hydrogen-Air Jet Flames

In order to study the stability of a lifted jet flame by nozzle-generated vortexes, we have developed a chemical explosive mode analysis (CEMA) to investigate the near-field structure of the stabilization region of a turbulent lifted hydrogen-air jet flame in a heated air co-flow, computed with three-dimensional direct numerical simulation (DNS). The simulation was performed with a detailed hydrogen–air mechanism and mixture-averaged transport properties at a jet Reynolds number of 11,000 with over 900 million grid points. Explosive chemical modes and their characteristic time scales, as well as the species involved, were identified from the Jacobian matrix of the chemical source terms for species and temperature. We have defined an explosion index for explosive modes, indicating the

participation of species and temperature in the explosion process. Radical and thermal runaway can consequently be distinguished. CEMA of the lifted flame shows the existence of two premixed flame fronts, which are difficult to detect with conventional methods. The upstream fork preceding the two flame fronts thereby identifies the stabilization point. We have determined a Damköhler number based on the time scale of the chemical explosive mode and the local instantaneous scalar dissipation rate, to show the role of auto-ignition in affecting the stabilization point and in stabilizing the flame.

This work is in press at the *Journal of Fluid Mechanics* under the title: "Three-dimensional direct numerical simulation of turbulent lifted hydrogen/air jet flame in heated co-flow: a chemical explosive mode analysis", see Publication #5.

Archival Publications

The following papers report work sponsored by the present program.

1. P. Zhang and C. K. Law, "Bouncing and coalescence in head-on droplet collision with large deformation", submitted for publication in *Journal of Fluid Mechanics*.

2. H. Q. Zhang and C. K. Law, "Effects of temporally varying liquid-phase mass diffusivity in multicomponent droplet gasification", *Combustion and Flam*e **153**, 593–602 (2008).

3. X. S. Wu and C. K. Law, "Flame-acoustic resonance initiated by vortical disturbances", *Journal of Fluid Mechanics* **634**, 321–357 (2009).

4. V. Akkerman, C. K. Law and V. Bychkov, "Self-similar accelerative propagation of expanding wrinkled flames and explosion triggering", submitted for publication in *Proceedings of the Combustion Institute*.

5. T. F. Lu, C. S. Yoo, J. H. Chen and C. K. Law, "Three-dimensional direct numerical simulation of turbulent lifted hydrogen/air jet flame in heated co-flow: a chemical explosive mode analysis", *Journal of Fluid Mechanics*, in press.

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- V’yacheslav Akkerman, Research Staff
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